

Book Reviews

Data analysis for chemists, David Livingstone, Oxford Science Publications, Oxford University Press, UK, 1995, xvi + 239 pp., price UK£40.00. ISBN 0-19-855728-0

The subtitle to this book, 'Applications to QSAR and Chemical Product Design', gives a better indication of its contents. Professor Livingstone is a leading authority in this research area, having formerly managed the QSAR section at SmithKline Beecham Pharmaceuticals and having made a number of seminal contributions to advance the research in this field. The book is a successful practical account of how to do QSAR, particularly, but not entirely, with respect to medicinal chemistry. In my estimation, the book deserves to be on the desk of all scientists and students working with QSAR methods.

In some chapters, the book uses boxing devices for supplementary material which need not be read by an informed student but would be very useful for a newcomer. The book is based on the need for a fair knowledge of statistics and leads the reader through a number of examples, with sufficient tables of data and figures, to allow a good appreciation of the problem. My guess is that students who have read this book carefully will not encounter much difficulty when putting the methods into practice. The author is at pains to point out the many pitfalls that may plague an unthinking application to molecular design.

Chapter 1 begins with the concept that various molecular properties can be quantified as molecular parameters, and that these parameters may be related to the activity within a series of compounds. The fundamental problems which face the practitioner of QSAR are centred on a proper experimental design. In the past, many QSARs have subsequently been found to be flawed because the statistical design was inadequate. Chapter 2 will remind readers of the constant need for vigilance against weak experimental design; students would be well advised to discuss these problems in tutorials. The need for transforming data into a standardised form is covered in chapter 3 where the problem of multicollinearity is highlighted. Chapter 4 emphasises the need to examine the data by certain display methods. Pictures of data patterns give the user an intuitive feel for relationships, whether data show clustering, perturbation by outliers and other odd sta-

tistical quirks which can easily be missed if not inspected. In chapter 5 we are treated to a discussion of topics grouped as Unsupervised Learning; factor analysis and cluster analysis are handled well and significance for clusters is explained. Regression analysis, often a topic which students find difficult for multiple regression problems, is dealt with painlessly. In my opinion chapter 6 is probably the best 25 pages that can be found on the subject. Discriminant analysis and partial least squares form the content of chapter 7. Multivariate analysis is described in chapter 8 and covers principal components and factor analysis, cluster analysis, spectral-map analysis and models for dependent and independent data. The last chapter delves into new methods of artificial intelligence applied to data analysis. An area in which the author has been pre-eminent is the application of neural networks to deriving functional relationships between structure and activity. Perhaps modesty has restricted the length of this section; I would have preferred a little more, owing to my optimism about that area of research.

I am very positive about the value of this book. It is impeccably written and will be my choice to recommend to students learning about QSAR.

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Allelopathy: organisms, processes, and applications, ed. Inderjit, K. M. M. Dakshini & F. A. Einhellig, American Chemical Society, Washington DC, 1995, x + 381 pp., price US\$99.95. ISBN 0 8412 3061 7

In its simplest sense, allelopathy may be defined as the release of a chemical by one plant or micro-organism that inhibits the growth of nearby plants or micro-organisms and so reduces competition for space and resources for growth. More recently it is regarded as a complex of subtle chemical communications that encompass the interactions of micro-organisms, insects and higher animals with the plant kingdom in natural or agricultural ecosystems.

We are now certain that micro-organisms and plants release volatile organic compounds from their surfaces and leachates from leaves and roots, and other allelochemicals are released into the environment on their